Data-Driven Materials Simulations and Experiments

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Data-driven approaches, particularly machine-learning methods, have seen strong uptake across the natural sciences, including materials science, over the last decade. After a brief overview of my group's activities in data-driven materials science, I will focus on two of our research directions, accelerated molecular dynamics simulations and autonomous laboratories.

Ultra-fast machine-learning interatomic potentials (UFPs; Xie, Rupp, Hennig, npj Comput. Mater., 2023) combine the computational efficiency of traditional empirical potentials with an accuracy close to that of electronic-structure methods. This often enables molecular dynamics simulations at extended length and time scales that agree with experimental observations. I will present the UFP approach (effective two- and three-body potentials in a cubic B-spline basis with second-order-regularised linear regression), highlight independent applications (peritectic decomposition of SiC, epitaxial growth of MoS2, Li diffusion in solid-state electrolytes), and comment on the applicability and validation of UFPs.

Donor-acceptor conjugated polymers based on polycyclic aromatic compounds are a materials class that offers finely tunable electronic properties and high conductivity, e.g., for photocatalytic water splitting and CO2 reduction. However, many candidate polymers exist, and their solution-based synthesis suffers from solubility and aggregation issues. To overcome these challenges, we combine an automated oxidative chemical vapour deposition setup for the synthesis of thin polymer films with experiment planning via Bayesian optimisation with Gaussian process regression. This approach reduced the duration of experimental campaigns from months to weeks and yielded a three-fold improvement in conductivity.